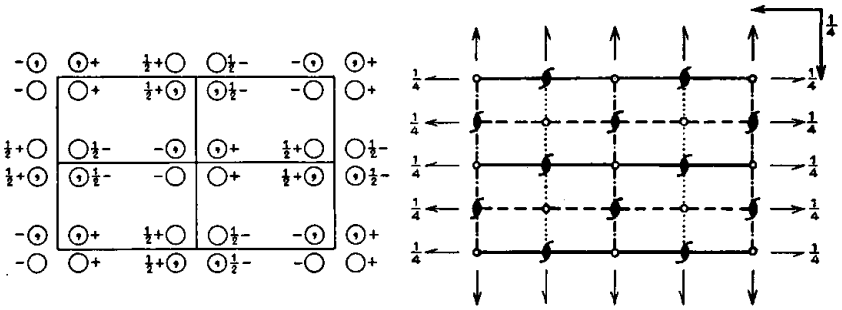
高温超伝導体 La_2CuO_4 の結晶構造データ

Composition La2 Cu O3.88
Unit Cell 5.360(1) 13.181(6) 5.393(3) 90. 90. 90. D(calc) 7.03 g/cm3
Vol 381.02 Z 4 Space Group C m c a
SG Number 64 Cryst Sys orthorhombic R Value 0.0333

Atom	#	OX	SITE	x	y	z	SOF
La	1	+3	8 f	0	0.36105(4)	0.0046(2)	1.
Cu	1	+1.76	4 a	0	0	0	1.
O	1	-2	8 f	0	0.18290(8)	-.0743(5)	0.943(4)
O	2	-2	8 e	0.25	-.0251(1)	0.75	0.995(3)

Lbl	Type	U11	U22	U33	U12	U13	U23
La1	La3+	0.0091(6)	0.0053(1)	0.0053(5)	0	0	0.004(3)
Cu1	Cu2+	0.0001(7)	0.0099(2)	0.0066(8)	0	0	-.0002(5)
O1	O2-	0.024(1)	0.0057(3)	0.019(1)	0	0	-.0014(5)
O2	O2-	0.0050(7)	0.0165(4)	0.0067(8)	0	0.0020(2)	0

Orthorhombic $m\,m\,m$ $C\,2/m\,2/c\,2_1/a$ No. 64 $Cmca$ D_{2h}^{18}

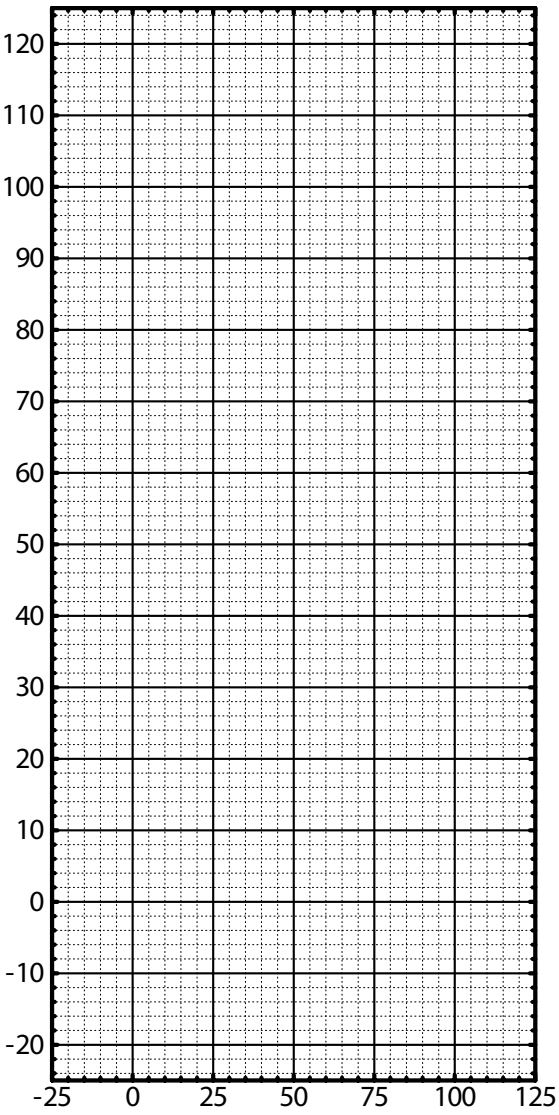


Origin at centre (2/*m*)

Number of positions, Wyckoff notation, and point symmetry			Co-ordinates of equivalent positions	Conditions limiting possible reflections
			(0,0,0; $\frac{1}{2},\frac{1}{2},0$)+	
16	*g*	1	x,y,z; $\bar{x},\bar{y},\bar{z}$;	General: hkl: $h+k=2n$; $0kl$: $(k=2n)$; $h0l$: $l=2n$; $(h=2n)$; $hk0$: $h=2n$; $(k=2n)$; $h00$: $(h=2n)$; $0k0$: $(k=2n)$; $00l$: $(l=2n)$
8	*f*	*m*	0,y,z;	Special: as above, plus no extra conditions
8	*e*	2	$\frac{1}{4},y,\frac{1}{4}$;	hkl: $h=2n$; $(k=2n)$
8	*d*	2	x,0,0;	hkl: $k+l=2n$; $(l+h=2n)$
8	*c*	$\bar{1}$	$\frac{1}{4},\frac{1}{4},0$;	hkl: $h,l=2n$; $(k=2n)$
4	*b*	2/*m*	$\frac{1}{2}$,0,0;	hkl: $k+l=2n$; $(l+h=2n)$
4	*a*	2/*m*	0,0,0;	

Symmetry of special projections

(001) *pmm*; $a'=a/2$, $b'=b/2$ (100) *pgm*; $b'=b/2$, $c'=c$ (010) *pmm*; $c'=c/2$, $a'=a/2$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25
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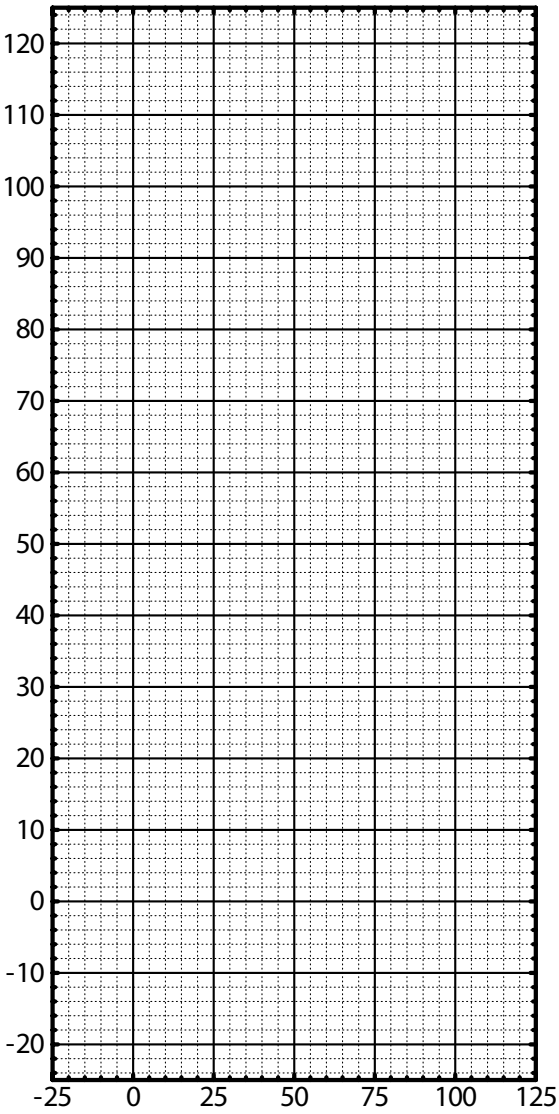
125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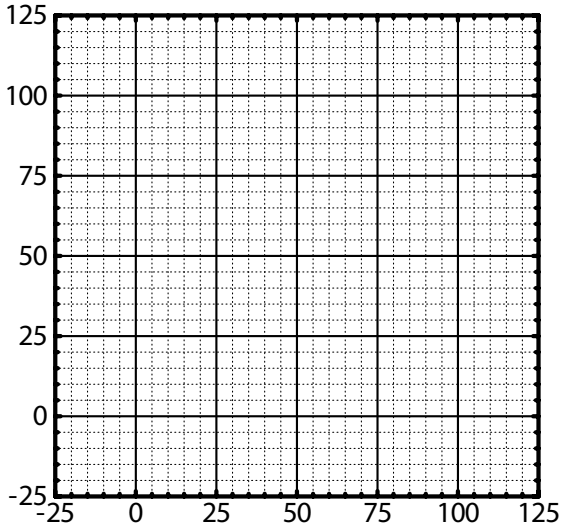
75
100
125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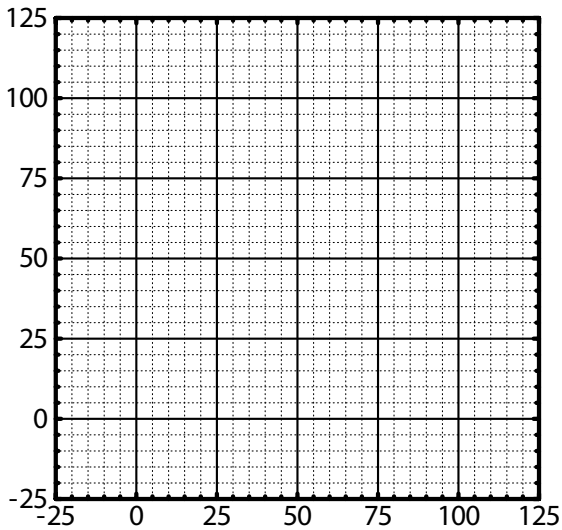
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